

São Paulo ICTP/TWAS Advanced School on Computational Materials Science for Energy and Environmental Applications

5 – 16 September 2011

(Santo André - Brazil)

The Abdus Salam International Centre for Theoretical Physics is organizing in collaboration with the Fundação de Amparo à Pesquisa do Estado de São Paulo, Brazil (FAPESP), the Universidade Federal do ABC (UFABC), the CNR-IOM Democritos Simulation Center, Trieste, and the Academy of Sciences for the Developing World (TWAS) an *Advanced School on Computational Materials Science for Energy and Environmental Applications* to be held in Santo André, Brazil from 5 to 16 September 2011.

The necessity to satisfy environmentally friendly the demand of energy in the World has lead to increasing interest in the use of renewable and clean sources of energy. At the same time, new sources and methodologies are needed to efficiently explore alternative fossil fuels and biofuels. These energy and environmental issues are particularly important for Latin America and Africa continents due to the technological gap, specially the use of hydrogen and solar energy. In addition, advanced technologies are needed to better explore oil and biofuel resources, in which Latin America and Africa, are large producers, in particular Brazil. The School will provide an overview on the advanced computational methods to address the problem of materials for energy and environmental applications. Topics will include: Functionals development and modeling dispersion forces, Electrical and thermal transport, Large scale DFT and TDDFT, Interatomic potentials development, Integrated and Multi-scale modeling, Theoretical spectroscopy, Ab-initio thermodynamics, Catalysis and Materials for energy and environmental applications. The School will include a series of advanced talks covering the latest developments as well as a series of hands-on tutorials based on public licence computer codes, high-performance computing and classical molecular dynamics and Monte Carlo codes.

Participation

Applicants from all countries that are members of the United Nations, UNESCO or IAEA may attend. As the Workshop will be conducted in English, participants should have an adequate working knowledge of this language. Limited funds are available for participants who are not more than 45 years old. Such support is available only to those attending the entire activity. *There is no registration fee.*

HOW TO APPLY FOR PARTICIPATION

The Online Application can be accessed at the activity website: <http://agenda.ictp.it/smr.php?2277>. Comprehensive instructions will guide you step-by-step on how to fill out and submit the application form. Kindly send all file attachments in Word or Acrobat format.

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Application DEADLINES

or

**19 June 2011
(if requiring Visa)
15 July 2011
(if not requiring Visa)**

CO-SPONSORED BY:



Directors

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Lecturers include

*Alex Antonelli (Unicamp - Brazil)
Francesca Baletto (Kings College - UK)
Stefano Baroni (SISSA/Democritos - Italy)
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